

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.54

Global applicability domain: Inside

Local applicability domain index: 9.62e-01

Confidence level: 8.22e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4,4'-Dichlorobiphenyl</div> <div>Measured: 7.68</div> <div>Predicted: 7.38</div>	<div>Image not found</div> <div>2,2'-Dichlorobiphenyl</div> <div>Measured: 7.18</div> <div>Predicted: 7.38</div>	<div>Image not found</div> <div>2,4'-Dichlorobiphenyl</div> <div>Measured: 7.40</div> <div>Predicted: 7.38</div>
<div>Image not found</div> <div>1,2,3,4-Tetrachloronaphthalene</div> <div>Measured: 8.30</div> <div>Predicted: 8.41</div>		